SAND2016-8658C

Optimization under Uncertainty

— Scramjet and Power Grid —

Habib N. Najm

Sandia National Laboratories
Livermore, CA

SAMSI 2016-2017 Program on Optimization Opening Workshop
Research Triangle Park
Aug 29 – Sep 2, 2016

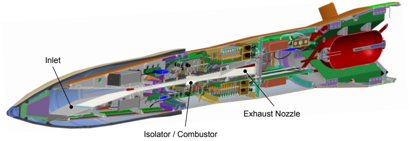
Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

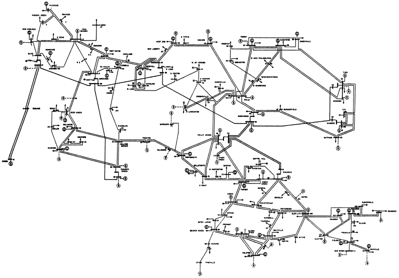
Outline

1. Introduction
2. Optimization of Scramjet Design
3. Optimization of Power Grid Operations
4. Closure

Introduction

- Practical engineered physical systems involve significant uncertainty
  - Model structure, parameters, inputs, operating conditions, . . .
- Hence the relevance of optimization under uncertainty (OUU)
- Two examples of our ongoing OUU work
- Scramjet combustor design
- Power grid operation





Scramjet OUU

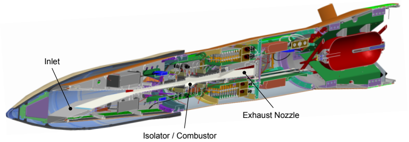
Joint work with

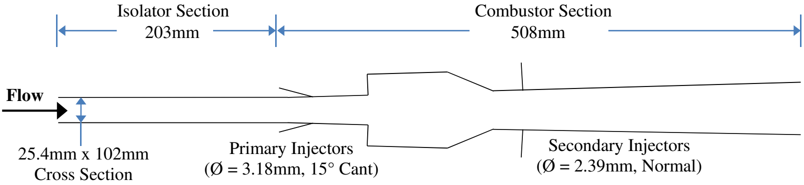
- Sandia National Labs:
  - Joe Oefelein, Guilhem Lacaze, Zachary Vane (LES-Comb.)
  - Khachik Sargsyan, Cosmin Safta, Xun Huan (UQ)
  - Mike Eldred (OUU)
- MIT:
  - Youssef Marzouk, Florian Augustin (OUU)

Work funded by DARPA EQUiPS program.

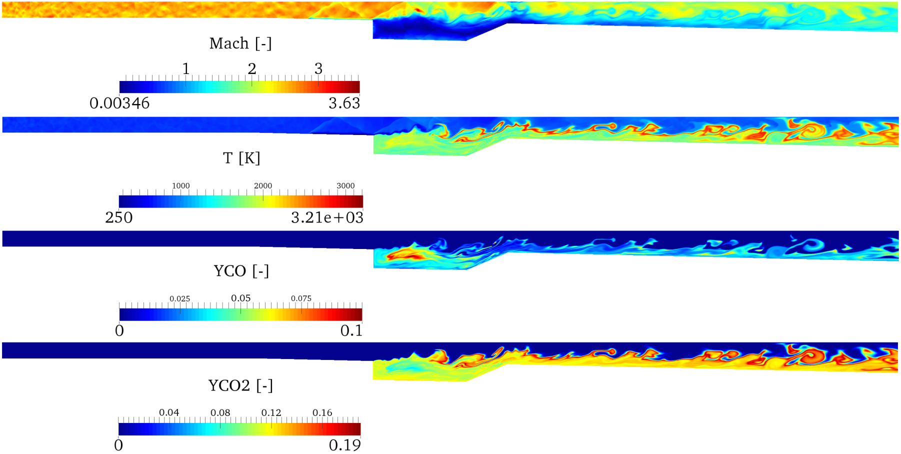
Scramjet Application

- 3D supersonic turbulent spray combustion system
- Optimization goals – examples:
  - Maximize specific thrust while ensuring stable combustion
  - ... and also minimize weight
  - etc
- Control variables: geometry and/or fuel injection details





Example flow pictures



Scramjet OUU Challenges and Mitigation

Challenges

- Model complexity and associated per-sample computational cost
  - Noisy objective function due to finite sample size in flow statistics
- No analytical gradients or Hessians
- High dimensionality in both random and design domains

Mitigation

- Rely on Multilevel Multifidelity (MLMF) methods
  - Multigrid optimization
  - Trust region model management (TRMM)
- Derivative free methods using local sparse surrogates
  - TRMM with gradient-based minimizers
  - Local fitted surrogates of QoIs over design+random space

$$R(\boldsymbol{\xi}, \mathbf{d}) = \sum_{k=0}^{P} \alpha_k \Psi_k(\boldsymbol{\xi}, \mathbf{d})$$

- Existing optimization+UQ libraries
  - DAKOTA – https://dakota.sandia.gov
  - (S)NOWPAC – https://bitbucket.org/fmaugust/nowpac

Preliminary results – SNOWPAC (MIT)

Problem formulation

$$\min \mathbb{E}[Z_\sigma]$$
$$\text{s.t.} \quad \mathbb{E}[M] \geq 2$$

- Z_σ: spatial standard deviation of mixture fraction close to outlet
- M: Mach number (spatial mean) close to outlet

Constraints on design + uncertain parameters

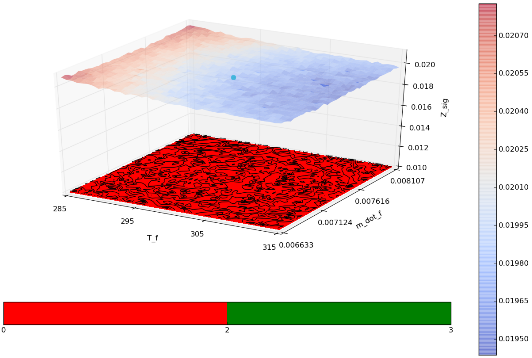
- $M_0 \in [2.259, 2.761]$
- $M_f \in [0.95, 1.05]$
- $T_f \in [285, 315]$
- $\dot{m}_f \in [6.633, 8.107] \cdot 10^{-3}$
- $T_0 \sim \mathcal{U}[1472.5, 1627.5]$
- $p_0 \sim \mathcal{U}[1.4061.554]$

Computational setup

- Use surrogate models from GSA as substitutes for LES code
- Use only 10 samples to approximate expected values

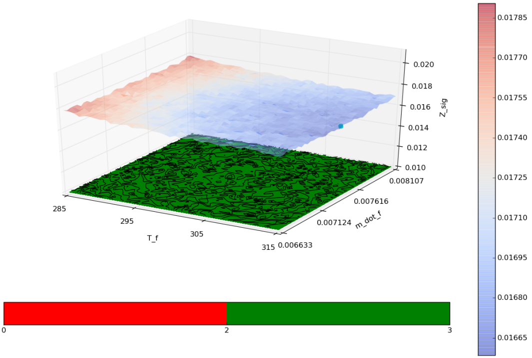
Optimization – Results

- $2D$ slice of $\mathbb{E}[Z_\sigma]$ and $\mathbb{E}[M]$ around **initial design** (cyan dot)
- Initial design **violates constraint** (i.e., yields $\mathbb{E}[M] < 2$)
- Objective and constraint **evaluations are noisy**



Optimization – Results

- $2D$ slice of $\mathbb{E}[Z_\sigma]$ and $\mathbb{E}[M]$ around **optimal design** (cyan dot)
- Optimal design **satisfies constraint** (i.e., yields $\mathbb{E}[M] \geq 2$)
- Minimization and finding a feasible design **despite noise**



Optimization of Power Grid Operations

Joint work with

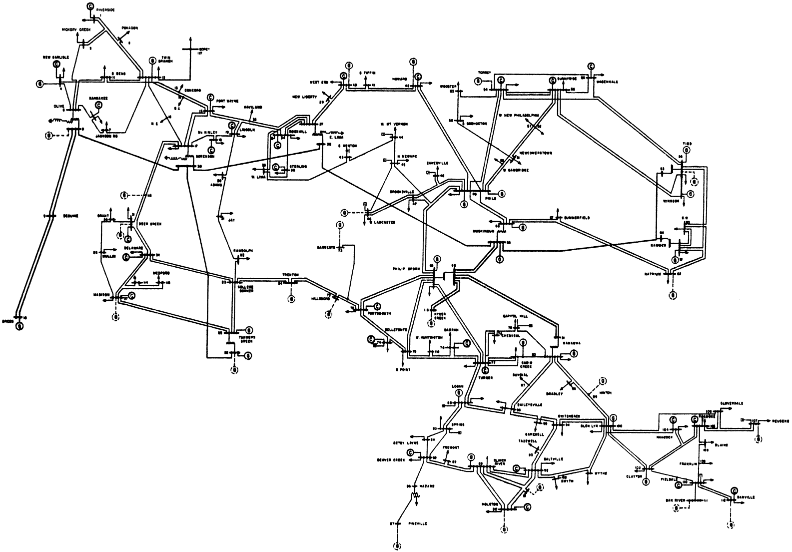
- At Sandia National Labs:
  - Cosmin Safta (UQ)
  - Richard Chen, Ali Pinar, Jianqiang Cheng, and Jean-Paul Watson (Optimization)

Work funded by the Sandia National Labs. LDRD program.

Power Grid Optimization under Uncertainty

- The electric power grid is a large complex system comprised of
  - Generators
    - Conventional power (coal, gas, hydro, nuclear, geothermal)
    - Alternative power (wind, solar, . . .)
  - Loads – Residential, industrial, . . .
  - Network – Transmission cables, hubs, . . .
- Conventional power plants are large and heterogeneous
  $\Rightarrow$ Starting up, power ramping, and shutting down involve significant time lags and operational constraints
- Optimal grid operation requires forward planning for generation power levels over a time scale of days – hourly time resolution
  1. Which power plants will be ON at which times
  2. What power levels will they be generating
- This has to be done given uncertainties in
  - Loads – predictable to some extent given historical data
  - Alternative power generation – higher level of uncertainty

A small benchmark 118-bus power grid system



Stochastic Power Grid Optimization Problem Structure

- Given time epochs $\{t_1, \ldots, t_T\}$
- Decision variables – given N generators:
  - Binary variables: ON/OFF indicators $x = \{x_1(t_k), \ldots, x_N(t_k)\}$
  - Continuous variables: Gen. power levels $Q = \{Q_1(t_k), \ldots, Q_N(t_k)\}$
- Constraints – physical constraints due to generators, lines, and loads
- Demand: $D = \{D_1(t_k), \ldots D_L(t_k)\}$ – L loads
- Objective: Minimize expected operational *Cost*
  - other measures – moments/statistics of uncertain cost
- Challenges
  - Two level Mixed integer optimization problem
    - Outer (integer) problem: Stochastic Unit Commitment
    - Inner problerm: Economic Dispatch
  - Large complex system – computational expense of cost evaluation
  - High dimensional – large # generators, loads, constraints
  - Uncertain demand
  - Uncertain alternative power generation

Stochastic optimization solution

- Need to evaluate moments of uncertain outputs given uncertain inputs – for evaluation of objective function
- Require joint probability density function on uncertain inputs over time
  - Correlations among uncertain inputs are important
  - Autocorrelation in time – stochastic process structure
- Conventional solution methods:
  - Evaluate expected cost via random sampling of uncertain inputs
  - Monte Carlo (MC) sampling in its many varieties – Quasi MC (QMC)
  - Advantage:
    - Robust performance given high-dimensional uncertain input
  - Disadvantage: low accuracy
- Recent work:
  - Functional representations of random variables / fields
  - Evaluate expectation integrals using sparse quadrature samples

Polynomial Chaos based Propagation of Uncertainty

- Polynomial Chaos expansion (PCE): $X = \sum_{k=0}^{\infty} x_k \Psi_k(\boldsymbol{\xi})$
  - A Fourier-like expansion of any random variable (with finite variance) in terms of orthogonal functions of a set of *iid* standard random variables
- Karhunen-Loéve expansion (KLE)
  - An L2-optimal expansion for a random field in terms of a set of uncorrelated random variables – covariance matrix eigenmodes
- Deal with functional representations of random variables/fields, rather than probability densities
- Given $X = \sum_k x_k \Psi_k(\boldsymbol{\xi})$, the coeffs. of $Y = f(X) \approx \sum_k y_k \Psi_k(\boldsymbol{\xi})$ can be found via Galerkin projection

$$y_k = \frac{\langle f \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{\langle \Psi_k^2 \rangle} \int f(X(\boldsymbol{\xi})) \Psi_k(\boldsymbol{\xi}) p_{\boldsymbol{\xi}}(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi}$$

- Efficient numerical integration via sparse quadrature
  - rather than Monte Carlo sampling

Stochastic Economic Dispatch

$$Q(\boldsymbol{x}, \boldsymbol{\xi}(\omega)) = \min_{\boldsymbol{f}, \boldsymbol{p} \geq \boldsymbol{0}, \boldsymbol{q} \geq \boldsymbol{0}, \boldsymbol{\theta}} \sum_{t \in T} \sum_{g \in G} c_g^P(p_g^t) + \sum_{t \in T} \sum_{i \in N} M q_i^t$$

s.t.

$$\sum_{r \in R_i} p_r^t(\boldsymbol{\xi}(\omega)) + \sum_{g \in G_i} p_g^t + \sum_{e \in E_{.i}} f_e^t - \sum_{e \in E_{i.}} f_e^t = D_i^t(\boldsymbol{\xi}(\omega)) - q_i^t,$$

$$B_e(\theta_i^t - \theta_j^t) - f_e^t = 0, \quad \forall e = (i,j), t$$

$$\underline{F}_e \leq f_e^t \leq \overline{F}_e, \quad \forall e, t$$

$$\underline{P}_g x_g^t \leq p_g^t \leq \overline{P}_g x_g^t, \quad \forall g, t$$

$$p_g^t - p_g^{t-1} \leq R_g^u x_g^{t-1} + S_g^u(x_g^t - x_g^{t-1}) + \overline{P}_g(1 - x_g^t), \quad \forall g, t$$

$$p_g^{t-1} - p_g^t \leq R_g^d x_g^t + S_g^d(x_g^{t-1} - x_g^t) + \overline{P}_g(1 - x_g^{t-1}), \quad \forall g, t$$

Consider uncertain renewables $p_r^t(\boldsymbol{\xi}(\omega))$ and demand $D_i^t(\boldsymbol{\xi}(\omega))$.

PCE for Q:

$$Q(x, \boldsymbol{\xi}) = \sum_k Q_k(x) \Psi_k(\boldsymbol{\xi})$$

Stochastic Unit Commitment

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & c^u(\boldsymbol{x}) + c^d(\boldsymbol{x}) + \overline{Q}(\boldsymbol{x}) \\ \text{s.t.} \quad & \boldsymbol{x} \in \mathcal{X}, \\ & \boldsymbol{x} \in \{0,1\}^{|G|\times|T|} \end{aligned}$$

- G and T: index sets of generating units and time periods
- $\mathcal{X}$ and $\boldsymbol{x}$: set of unit commitment constraints and vector of unit commitment decisions
- $c^u(\boldsymbol{x})$ and $c^d(\boldsymbol{x})$: generating unit start-up and shut-down costs
- $\overline{Q}(\boldsymbol{x})$: the expected generation cost

Compute

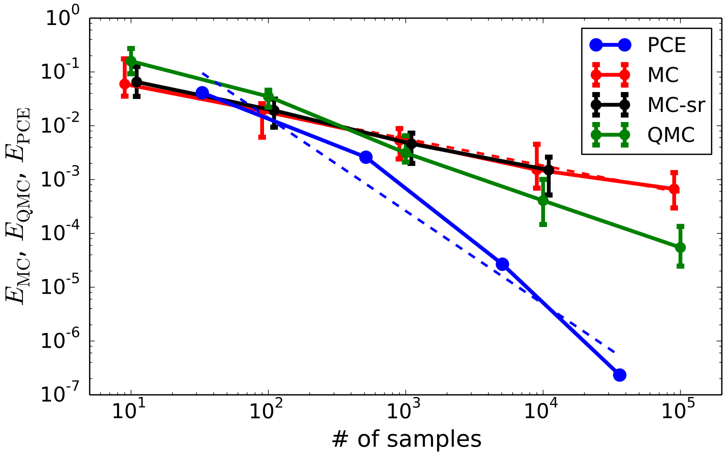
$$\overline{Q}(\boldsymbol{x}) = \langle Q(\boldsymbol{x},\boldsymbol{\xi})\rangle \equiv Q_0(\boldsymbol{x})|_{\text{PC Sp. Quad}} = \overline{Q}(\boldsymbol{x})|_{\text{MC}} \approx \frac{1}{|\mathcal{S}|}\sum_{s=1}^{|\mathcal{S}|} Q(\boldsymbol{x},\boldsymbol{\xi}_s)$$

using a finite number of renewable generation and load realizations (i.e., scenarios) $s \in \mathcal{S}$

Illustration on a Model Power Grid problem

- IEEE 118-bus system augmented with 3 wind farms
- Economic dispatch problem, with a specified set of ON generators
- 24-hr time horizon, 1-hr time epochs
- Uncertain power from each wind farm is a random field
  - Random field KLE based on empirical wind data
  - Correlation among two neighboring wind farms in longer-timescale random field structure – observed in data and accounted for in KLE structure
- Uncertain input thus represented with a 16 dimensional PCE
- Comparisons in computed $Q_0(x)$ among:
  - PC-sparse quadrature
  - MC
  - MC with scenario reduction
  - QMC – low discrepancy sequence

Error Convergence in Economic Dispatch Expected Cost



Convergence of error in estimation of $Q_0(x)$ for PCE, MC, MC-SR, QMC

Closure

- Highlighted two applications of optimization under uncertainty being worked on at Sandia
- Scramjet
  - Prohibitive computational costs
  - Focus on multifidelity multilevel strategies with TRMM and MG/Opt
  - Efficient estimation of local surrogates with controlled accuracy is key
- Power Grid
  - KLE enables low-dimensional representation of uncertain time-dependent wind power – Captures correlations
  - In 16D, PCE superior over MC/variants for accuracies $<1\%$
  - With higher dimensionality, global sensitivity analysis is useful for employing sparse lower-dimensional PCE constructions
  - Ongoing work on extension of PCE/Sparse-quadrature to the Unit Commitment problem